

10/513699

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PASSWORD:

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* * * * * Welcome to STN International * * * * *

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Classification Data
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NEWS 13 FEB 06 Patent sequence location (PSL) data added to USGENE
NEWS 14 FEB 10 COMPENDEX reloaded and enhanced
NEWS 15 FEB 11 WTEXTILES reloaded and enhanced
NEWS 16 FEB 19 New patent-examiner citations in 300,000 CA/CAPLUS
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precise author group fields and 2009 MeSH terms
NEWS 21 FEB 23 Three million new patent records blast AEROSPACE into
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NEWS 22 FEB 25 USGENE enhanced with patent family and legal status
display data from INPADOCDB
NEWS 23 MAR 06 INPADOCDB and INPAFAMDB enhanced with new display
formats

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,

<12/04/2007>

Erich Leese

10/513699

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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FILE 'HOME' ENTERED AT 16:23:34 ON 10 MAR 2009

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.44	0.44

FILE 'REGISTRY' ENTERED AT 16:24:30 ON 10 MAR 2009
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STRUCTURE FILE UPDATES:	9 MAR 2009	HIGHEST RN 1118246-54-0
DICTIONARY FILE UPDATES:	9 MAR 2009	HIGHEST RN 1118246-54-0

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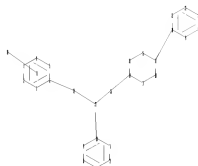
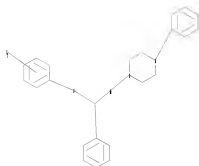
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\Stnexp\Queries\10594105restriction.str



```

chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
exact bonds :
10-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

```

G1:C,N

10/513699

G2:CF2,CF3,CC12,CC13,CBr2,CBr3,X

Match level :

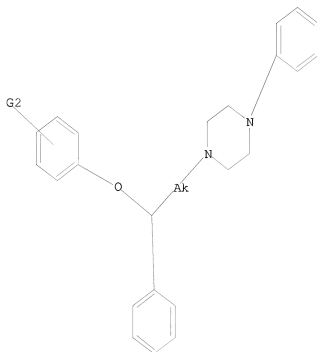
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 C,N

G2 CF2,CF3,CC12,CC13,CBr2,CBr3,X

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 16:25:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 10796 TO ITERATE

100.0% PROCESSED 10796 ITERATIONS

SEARCH TIME: 00.00.02

116 ANSWERS

<12/04/2007>

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10/513699

L2 116 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	186.36	186.80

FILE 'CAPLUS' ENTERED AT 16:25:35 ON 10 MAR 2009

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FILE COVERS 1907 - 10 Mar 2009 VOL 150 ISS 11

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=> s 12 full

L3 10 L2

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.50	188.30

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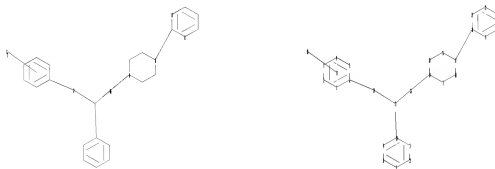
Please note that search-term pricing does apply when conducting SmartSELECT searches.

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<http://www.cas.org/support/stngen/stdoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10594105pyrimidine.str



```
chain nodes :
25 26 27 30
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24
chain bonds :
6-25 10-27 14-26 17-20 25-27 26-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24
```

<12/04/2007>

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10/513699

exact/norm bonds :
6-25 13-14 13-18 14-15 14-26 15-16 16-17 17-18 17-20 25-27 26-27
exact bonds :
10-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 19-20 19-24
20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 7 : 13 : 19 :

G1:C,N

G2:CF2,CF3,CC12,CC13,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 30:CLASS
31:Atom

L4 STRUCTURE UPLOADED

=> d 14

L4 HAS NO ANSWERS

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> d 14

L4 HAS NO ANSWERS

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 14 full

FULL SEARCH INITIATED 16:28:23 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 267 TO ITERATE

100.0% PROCESSED 267 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L5 6 SEA SSS FUL L4

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

185.88

374.18

<12/04/2007>

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=> s 15 full
L6 L5

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.00	376.18

FILE 'REGISTRY' ENTERED AT 16:30:33 ON 10 MAR 2009
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REGISTRY includes numerically searchable data for experimental and

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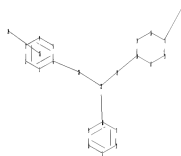
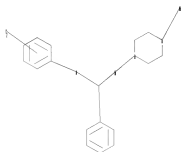
10/513699

predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10594105methyl.str



```
chain nodes :
19 20 21 22 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
6-20 10-22 14-21 17-19 20-22 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18
exact/norm bonds :
6-20 13-14 13-18 14-15 14-21 15-16 16-17 17-18 17-19 20-22 21-22
exact bonds :
10-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
```

<12/04/2007>

Erich Leese

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G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :

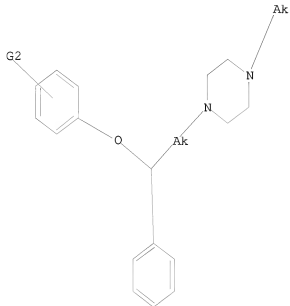
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 25:CLASS 26:Atom

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



G1 C,N

G2 CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Structure attributes must be viewed using STN Express query preparation.

=> s 17 full

FULL SEARCH INITIATED 16:31:06 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 69180 TO ITERATE

100.0% PROCESSED 69180 ITERATIONS

74 ANSWERS

SEARCH TIME: 00.00.02

<12/04/2007>

Erich Leese

10/513699

L8 74 SEA SSS FUL L7

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	185.88	562.06

FILE 'CAPLUS' ENTERED AT 16:31:15 ON 10 MAR 2009
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=> s l8 full
L9 8 L8

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.50	564.56

FILE 'REGISTRY' ENTERED AT 16:34:04 ON 10 MAR 2009
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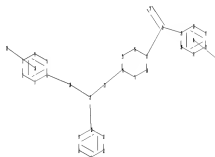
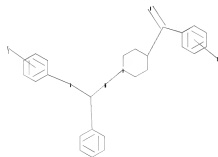
Please note that search-term pricing does apply when conducting SmartSELECT searches.

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=>

Uploading C:\Program Files\Stnexp\Queries\10594105piperidine.str



```
chain nodes :
19 20 21 22 25 33 34
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 27 28 29 30 31
32
chain bonds :
6-20 10-22 14-21 17-19 19-29 19-33 20-22 21-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14 13-18
14-15 15-16 16-17 17-18 27-28 27-32 28-29 29-30 30-31 31-32
exact/norm bonds :
6-20 13-14 13-18 14-15 14-21 15-16 16-17 17-18 19-33 20-22 21-22
```

10/513699

exact bonds :
10-22 17-19 19-29
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 27-28 27-32
28-29 29-30 30-31 31-32
isolated ring systems :
containing 27 :

G1:C,N

G2:CF2,CF3,CCl2,CCl3,CBr2,CBr3,X

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:CLASS 21:CLASS 22:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:CLASS 33:CLASS 34:CLASS 35:Atom

L10 STRUCTURE UPLOADED

=> s l10 full
FULL SEARCH INITIATED 16:34:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 847 TO ITERATE

100.0% PROCESSED 847 ITERATIONS 6 ANSWERS
SEARCH TIME: 00.00.01

L11 6 SEA SSS FUL L10

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 186.36 750.92

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FILE COVERS 1907 - 10 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 9 Mar 2009 (20090309/ED)

<12/04/2007>

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=> s l11 full

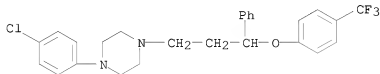
L12 2 L11

=> s l12 or l9 or l6 or l3

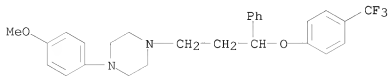
L13 16 L12 OR L9 OR L6 OR L3

=> d ibib abs hitstr tot

L13 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2008:803320 CAPLUS
 DOCUMENT NUMBER: 149:215113
 TITLE: Two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands
 AUTHOR(S): Weber, Karen C.; Honorio, Kathia M.; Andricopulo, Adriano D.; Da Silva, Alberico B. F.
 CORPORATE SOURCE: Instituto de Quimica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, 13560-970, Brazil
 SOURCE: Medicinal Chemistry (2008), 4(4), 328-335
 CODEN: MCEHAJ; ISSN: 1573-4064
 PUBLISHER: Bentham Science Publishers Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 5-HT1A receptor plays an important role in the delayed onset of antidepressant action of a class of selective serotonin reuptake inhibitors. Moreover, 5-HT1A receptor levels have been shown to be altered in patients suffering from major depression. In this work, hologram quant. structure-activity relationship (HQ SAR) studies were performed on a series of arylpiperazine compds. presenting affinity to the 5-HT1A receptor. The models were constructed with a training set of 70 compds. The most significant HQ SAR model ($q^2 = 0.81$, $r^2 = 0.96$) was generated using atoms, bonds, connections, chirality, and donor and acceptor as fragment distinction, with fragment size of 6-9. Predictions for an external test set containing 20 compds. are in good agreement with exptl. results showing the robustness of the model. Addnl., useful information can be obtained from the 2D contribution maps.
 IT 328248-15-3 328248-21-1 328248-23-3
 328248-24-4 328248-30-2 328248-36-8
 753439-74-6 767277-20-3 777843-82-0
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (two-dimensional QSAR studies on arylpiperazines as high-affinity 5-HT1A receptor ligands)
 RN 328248-15-3 CAPLUS
 CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



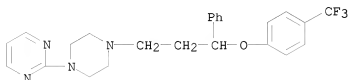
RN 328248-21-1 CAPLUS
 CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



10/513699

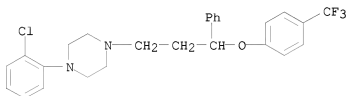
RN 328248-23-3 CAPLUS

CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



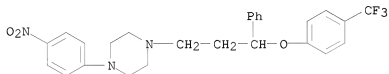
RN 328248-24-4 CAPLUS

CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



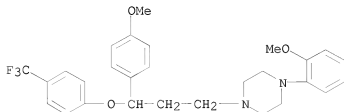
RN 328248-30-2 CAPLUS

CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-36-8 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

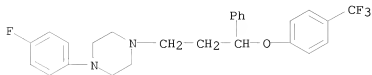


RN 753439-74-6 CAPLUS

CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-

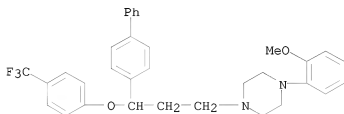
10/513699

(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



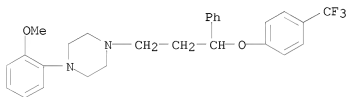
RN 767277-20-3 CAPLUS

CN Piperazine, 1-([3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl))- (CA INDEX NAME)



RN 777843-82-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

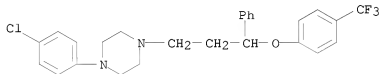


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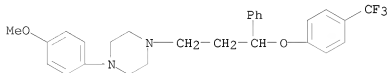
31

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

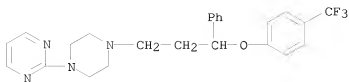
L13 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2008:767635 CAPLUS
 DOCUMENT NUMBER: 149:324283
 TITLE: Quantitative structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method
 AUTHOR(S): Kuz'min, V. E.; Polischuk, P. G.; Artemenko, A. G.; Makan, S. Yu.; Andronati, S. A.
 CORPORATE SOURCE: A.V. Bogatsky Physical-Chemical Institute, National Academy of Sciences of Ukraine, Odessa, Ukraine
 SOURCE: SAR and QSAR in Environmental Research (2008), 19(3-4), 213-244
 CODEN: SQERED; ISSN: 1062-936X
 PUBLISHER: Taylor & Francis Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The influence of mol. structure of 346 ligands on their affinity for 5-HT1A receptors was investigated. It was shown that the effectiveness of the proposed novel approach for interpretation of decision tree models compared favorably with the PLS method. In the context of the proposed approach, mol. fragments and their values of the relative influence on the affinity for 5-HT1A receptors were defined.
 IT 328248-15-3 328248-21-1 328248-23-3
 328248-24-4 328248-30-2 328248-36-8
 753439-74-6 767277-20-3 777843-82-0
 RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study)
 (quant. structure-affinity relationship of 5-HT1A receptor ligands by the classification tree method)
 RN 328248-15-3 CAPLUS
 CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-21-1 CAPLUS
 CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

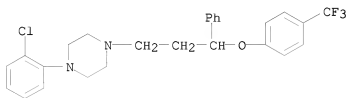


RN 328248-23-3 CAPLUS
 CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



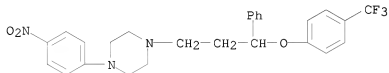
RN 328248-24-4 CAPLUS

CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



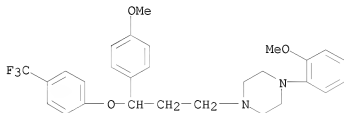
RN 328248-30-2 CAPLUS

CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-36-8 CAPLUS

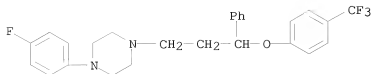
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 753439-74-6 CAPLUS

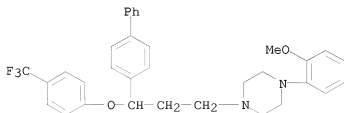
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

10/513699



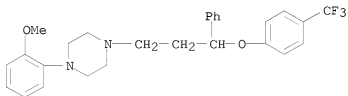
RN 767277-20-3 CAPLUS

CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 777843-82-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



REFERENCE COUNT:

25

THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2008:232006 CAPLUS

DOCUMENT NUMBER: 148:440268

TITLE: A chemometric study of the 5-HT1A receptor affinities presented by arylpiperazine compounds

AUTHOR(S): Weber, Karen C.; da Silva, Alberico B. F.

CORPORATE SOURCE: Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, 13566-590, Brazil

SOURCE: European Journal of Medicinal Chemistry (2008), 43(2), 364-372

CODEN: EJMCAS; ISSN: 0223-5234

PUBLISHER: Elsevier Masson SAS

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Arylpiperazine compds. are promising 5-HT1A receptor ligands that can contribute for accelerating the onset of therapeutic effect of selective serotonin reuptake inhibitors. In the present work, the chemometric methods HCA, PCA, KNN, SIMCA and PLS were employed in order to obtain SAR and QSAR models relating the structures of arylpiperazine compds. to their 5-HT1A receptor affinities. A training set of 52 compds. was used to construct the models and the best ones were obtained with nine topol. descriptors. The classification and regression models were externally validated by means of predictions for a test set of 14 compds. and have presented good quality, as verified by the correctness of classifications, in the case of pattern recognition studies, and by the high correlation coeffs. ($q^2 = 0.76$, $r^2 = 0.83$) and small prediction errors for the PLS regression. Since the results are in good agreement with previous SAR studies, we can suggest that these findings can help in the search for 5-HT1A receptor ligands that are able to improve antidepressant treatment.

IT 328248-21-1 328248-23-3 328248-24-4

328248-30-2 328248-36-8 753439-74-6

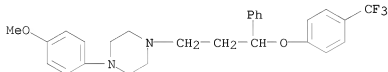
767277-20-3 777843-82-0

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(chemometric study of 5-HT1A receptor affinities presented by arylpiperazine compds. as possible antidepressants)

RN 328248-21-1 CAPLUS

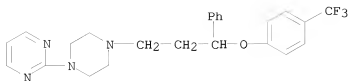
CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-23-3 CAPLUS

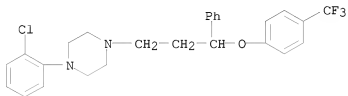
CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)

10/513699



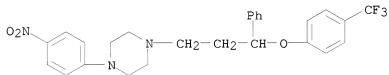
RN 328248-24-4 CAPLUS

CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



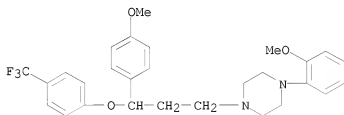
RN 328248-30-2 CAPLUS

CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-36-8 CAPLUS

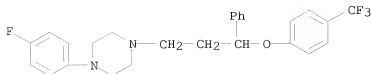
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 753439-74-6 CAPLUS

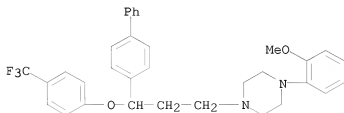
CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

10/513699



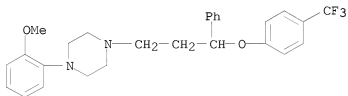
RN 767277-20-3 CAPLUS

CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 777843-82-0 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

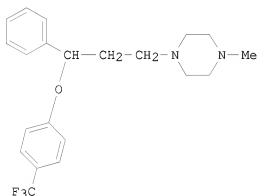


REFERENCE COUNT:

35

THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2006:847178 CAPLUS
 DOCUMENT NUMBER: 145:410017
 TITLE: Synthesis of benzenepropanamine analogues as non-detergent spermicides with antitrichomonas and anticandida activities
 AUTHOR(S): Kumar, S. T. V. S. Kiran; Sharma, Vishnu Lal; Kumar, Manish; Shukla, Praveen Kumar; Tiwari, Pratibha; Jain, Rajeev Kumar; Maikhuri, Jagdamba Prasad; Singh, Divya; Gupta, Gopal; Singh, Man Mohan
 CORPORATE SOURCE: Division of Medicinal and Process Chemistry, Central Drug Research Institute, Lucknow, 226001, India
 SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(19), 6593-6600
 CODEN: BMECEP; ISSN: 0968-0896
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 145:410017
 GI



I

- AB Fifteen analogs of benzenepropanamine were synthesized and evaluated for their spermicidal as well as microbicidal activities against *Trichomonas vaginalis* and *Candida* spp. Several compds. showed appreciable dual activities. Compound I exhibited good spermicidal (MEC = 0.1%) along with substantial anticandidal (MIC = 0.05%) activities, while compds. 3 and 6 showed significant microbicidal activities with moderate spermicidal effect. The SAR of these structures is being discussed here in this communication. It is concluded that suitable structural modifications in this class of compds. at 3-amino position may lead to a potent spermicide with associated microbicidal activity.
- IT 911811-07-9P 911811-08-0P 911811-09-1P
 911811-11-5P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

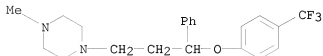
10/513699

(Uses)

(benzenepropanamine analogs as non-detergent spermicides with antitrichomonas and anticanidada activities)

RN 911811-07-9 CAPLUS

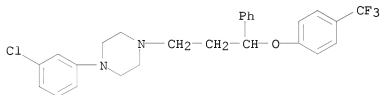
CN Piperazine, 1-methyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

RN 911811-08-0 CAPLUS

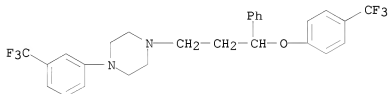
CN Piperazine, 1-(3-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 911811-09-1 CAPLUS

CN Piperazine, 1-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



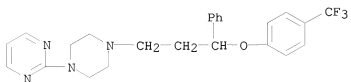
● HCl

RN 911811-11-5 CAPLUS

CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-

10/513699

piperaziny]-, hydrochloride (1:2) (CA INDEX NAME)



● 2 HCl

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1289687 CAPLUS

DOCUMENT NUMBER: 144:51568

TITLE: Preparation of substituted 2-quinolyl-oxazoles and their heterocyclic analogs useful as pde4 inhibitors

INVENTOR(S): Kuang, Rongze; Blythin, David; Shih, Neng-Yang; Shue, Ho-Jane; Chen, Xiao; Cao, Jianhua; Gu, Danlin; Huang, Ying; Schwerdt, John H.; Ting, Pauline C.; Wong, Shing-Chun; Xiao, Li

PATENT ASSIGNEE(S): Schering Corporation, USA

SOURCE: PCT Int. Appl., 233 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

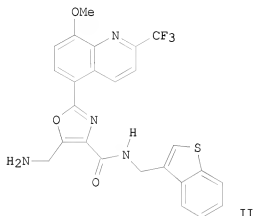
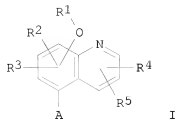
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005116009	A1	20051208	WO 2005-US17134	20050516
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005247906	A1	20051208	AU 2005-247906	20050516
CA 2565599	A1	20051208	CA 2005-2565599	20050516
US 20060106062	A1	20060518	US 2005-130359	20050516
EP 1758883	A1	20070307	EP 2005-750076	20050516
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
CN 1984901	A	20070620	CN 2005-80023666	20050516
BR 2005011295	A	20071204	BR 2005-11295	20050516
JP 2007537300	T	20071220	JP 2007-513471	20050516
TW 286475	B	20070911	TW 2005-94115924	20050517
MX 2006013414	A	20070123	MX 2006-13414	20061117
KR 2007013306	A	20070130	KR 2006-724186	20061117
IN 2006CN04254	A	20070629	IN 2006-CN4254	20061117
NO 2006005830	A	20070216	NO 2006-5830	20061215
PRIORITY APPLN. INFO.:			US 2004-572266P	P 20040518
			WO 2005-US17134	W 20050516

OTHER SOURCE(S): CASREACT 144:51568; MARPAT 144:51568

GI



AB Title compds. I [R1 = H, alkyl, cycloalkyl; R2, R3 and R5 independently = H or halo; R4 = H, halo, alkyl, etc.; A = substituted oxazolyl, imidazole, thiazole or pyrrole], and their pharmaceutically acceptable salts, are prepared and disclosed as pde4 inhibitors. Thus, e.g., II was prepared in a multistep synthesis from 2-trifluoromethyl-8-methoxyquinolin-5-yl carboxylic acid. In PDE4 assays, selected compds. possessed IC50 values ranging from 0.01-1.8 nM. Also claimed are pharmaceutical compns., the use of the compds. as PDE4 inhibitors, and combinations with other actives.

IT 871009-78-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

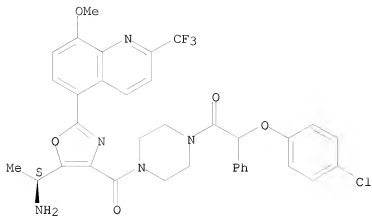
(preparation of substituted quinoloxazoles and their heterocyclic analogs useful as PDE4 inhibitors)

RN 871009-78-8 CAPLUS

CN Ethanone, 1-[4-[[5-[(1S)-1-aminoethyl]-2-[8-methoxy-2-(trifluoromethyl)-5-quinolinyl]-4-oxazolyl]carbonyl]-1-piperazinyl]-2-(4-chlorophenoxy)-2-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.

10/513699



● HCl

REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1143268 CAPLUS

DOCUMENT NUMBER: 144:63874

TITLE: Design and synthesis of long-chain arylpiperazines with mixed affinity for serotonin transporter (SERT) and 5-HT1A receptor

AUTHOR(S): Perrone, Roberto; Berardi, Francesco; Colabufo, Nicola A.; Lacivita, Enza; Larizza, Carmela; Leopoldo, Marcello; Tortorella, Vincenzo

CORPORATE SOURCE: Dipartimento Farmaco-Chimico, Universita degli Studi di Bari, Bari, 70125, Italy

SOURCE: Journal of Pharmacy and Pharmacology (2005), 57(10), 1319-1327

CODEN: JPPMAB; ISSN: 0022-3573

PUBLISHER: Pharmaceutical Press

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:63874

AB A new generation of antidepressant agents could be represented by compds. with mixed activity as serotonin transporter (SERT) inhibitors and 5-HT1A receptor antagonists. We report here on the synthesis and evaluation of SERT and 5-HT1A receptor affinity of long-chain arylpiperazines obtained either by modifying 6-nitroquipazine into a long-chain arylpiperazine or by inserting a modified 6-nitroquipazine moiety or other structures endowed with SERT affinity into a long-chain arylpiperazine with 5-HT1A affinity. Among the compds. studied, 2-[4-(2-methoxyphenyl)piperazin-1-yl]-N-(6-nitro-2-quinolyl)ethylamine (21) and 1-(5-bromo-1,2,3,4-tetrahydronaphthalen-1-yl)-3-[4-(2-methoxyphenyl)-piperazin-1-yl]-1-propanone (24) showed good affinity values for SERT and 5-HT1A receptors (SERT: Ki (inhibition constant) = 71.8 and 62.8 nM; 5-HT1A Ki = 14.2 and 0.82 nM, resp.).

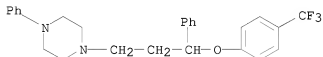
IT 871739-17-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(aryl)piperazines with mixed affinity for serotonin transporter and 5-HT1A receptor)

RN 871739-17-2 CAPLUS

CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

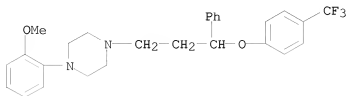
IT 777843-82-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(aryl)piperazines with mixed affinity for serotonin transporter and

10/513699

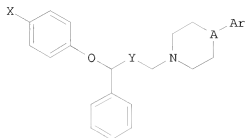
5-HT1A receptor)
RN 777843-82-0 CAPLUS
CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



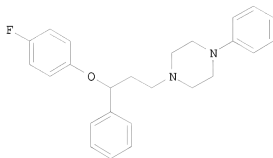
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:1103625 CAPLUS
 DOCUMENT NUMBER: 143:387060
 TITLE: Preparation of piperazine or piperidine derivatives as
 serotonin reuptake inhibitors
 INVENTOR(S): Pinney, Kevin G.; Miranda, Maria Graciela; Dorsey,
 James Michael
 PATENT ASSIGNEE(S): Baylor University, USA
 SOURCE: PCT Int. Appl., 52 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005094896	A2	20051013	WO 2005-US10356	20050328
WO 2005094896	A3	20070503		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AP, EA, EP, OA			
EP 1732610	A2	20061220	EP 2005-730778	20050328
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU			
US 20080132514	A1	20080605	US 2007-594105	20070921
PRIORITY APPLN. INFO.:			US 2004-557069P	P 20040326
			WO 2005-US10356	W 20050328
OTHER SOURCE(S):	CASREACT 143:387060; MARPAT 143:387060			
GI				



I



II

AB Title compds. I [X = F or CF₃; Y = (CH₂)_n; n = 0-1; A = N or C; Ar = aryl] and their pharmaceutically acceptable salts, are prepared and disclosed as serotonin reuptake inhibitors. Thus, e.g., II was prepared by reduction of 1-phenyl-3-(4-phenyl-piperazin-1-yl)-propan-1-ol (preparation given) using sodium borohydride followed by coupling with 4-fluorophenol. The ability of I to inhibit [3H]5-HT uptake was evaluated using liquid scintillation spectroscopy and it was revealed that selected compds. of the invention possessed IC₅₀ values in the range of 1.45 up to 9.56 μM. I as serotonin reuptake inhibitors should prove useful in the treatment of depression. Pharmaceutical composition comprising I are disclosed.

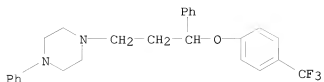
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 691872-60-3P 691872-62-5P 691872-64-7P
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 866548-23-4P 866548-24-5P 866548-25-6P
 866548-26-7P 866548-27-8P 866548-28-9P
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 866548-32-5P 866548-33-6P 866548-34-7P
 866548-35-8P 866548-36-9P 866548-37-0P
 866548-38-1P 866548-39-2P 866548-40-5P
 866548-41-6P 866548-42-7P 866548-43-8P
 866548-44-9P 866548-45-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperazine or piperidine derivs. as serotonin reuptake inhibitors)

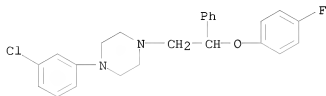
RN 158545-85-8 CAPLUS

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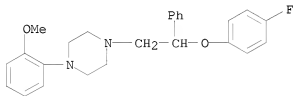
RN 691872-56-7 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



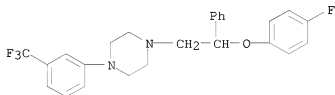
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



RN 691872-60-3 CAPLUS

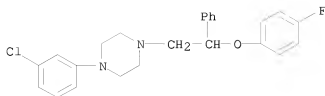
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



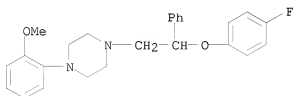
RN 691872-62-5 CAPLUS

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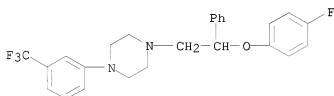
10/513699



RN 691872-64-7 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)

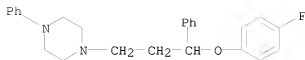


RN 691872-66-9 CAPLUS
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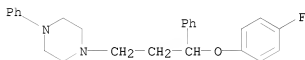


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CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl- (CA INDEX NAME)

10/513699

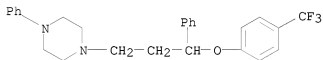


RN 866548-22-3 CAPLUS
CN Piperazine, 1-[3-(4-fluorophenoxy)-3-phenylpropyl]-4-phenyl-,
hydrochloride (1:1) (CA INDEX NAME)



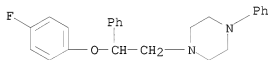
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RN 866548-23-4 CAPLUS
CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-,
hydrochloride (1:1) (CA INDEX NAME)



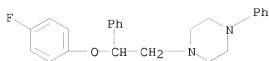
● HCl

RN 866548-24-5 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl- (CA INDEX
NAME)



RN 866548-25-6 CAPLUS
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-phenyl-, hydrochloride
(1:1) (CA INDEX NAME)

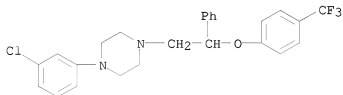
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● HCl

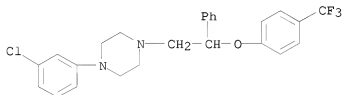
RN 866548-26-7 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)



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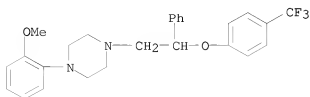
CN Piperazine, 1-(3-chlorophenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 866548-28-9 CAPLUS

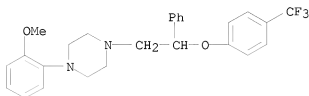
CN Piperazine, 1-(2-methoxyphenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]- (CA INDEX NAME)



10/513699

RN 866548-29-0 CAPLUS

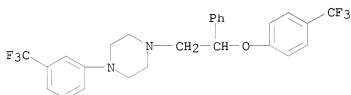
CN Piperazine, 1-(2-methoxyphenyl)-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

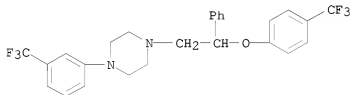
RN 866548-30-3 CAPLUS

CN Piperazine, 1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 866548-31-4 CAPLUS

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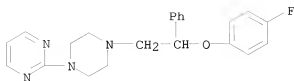


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RN 866548-32-5 CAPLUS

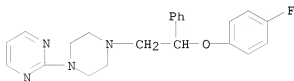
CN Pyrimidine, 2-[4-[2-(4-fluorophenoxy)-2-phenylethyl]-1-piperazinyl]- (CA INDEX NAME)

10/513699



RN 866548-33-6 CAPLUS

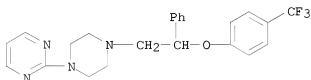
CN Pyrimidine, 2-[4-[2-(4-fluorophenoxy)-2-phenylethyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

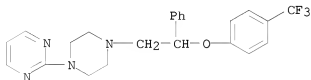
RN 866548-34-7 CAPLUS

CN Pyrimidine, 2-[4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-1-piperazinyl]- (CA INDEX NAME)



RN 866548-35-8 CAPLUS

CN Pyrimidine, 2-[4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-1-piperazinyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

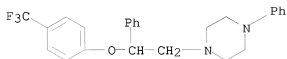
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<12/04/2007>

Erich Leese

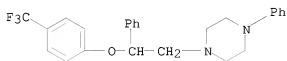
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CN Piperazine, 1-phenyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-
(CA INDEX NAME)



RN 866548-37-0 CAPLUS

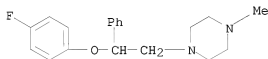
CN Piperazine, 1-phenyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-,
hydrochloride (1:1) (CA INDEX NAME)



● HCl

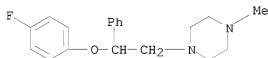
RN 866548-38-1 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-methyl- (CA INDEX
NAME)



RN 866548-39-2 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-methyl-, hydrochloride
(1:1) (CA INDEX NAME)

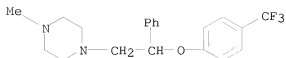


● HCl

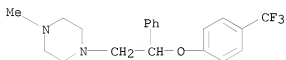
RN 866548-40-5 CAPLUS

CN Piperazine, 1-methyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-
(CA INDEX NAME)

10/513699

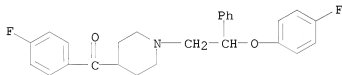


RN 866548-41-6 CAPLUS
CN Piperazine, 1-methyl-4-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-, hydrochloride (1:1) (CA INDEX NAME)

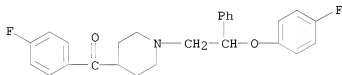


● HCl

RN 866548-42-7 CAPLUS
CN Methanone, [1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-piperidinyl] (4-fluorophenyl)- (CA INDEX NAME)



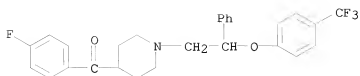
RN 866548-43-8 CAPLUS
CN Methanone, [1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-piperidinyl] (4-fluorophenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

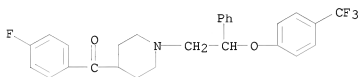
RN 866548-44-9 CAPLUS
CN Methanone, (4-fluorophenyl) [1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-piperidinyl]- (CA INDEX NAME)

10/513699



RN 866548-45-0 CAPLUS

CN Methanone, (4-fluorophenyl) [1-[2-phenyl-2-[4-(trifluoromethyl)phenoxy]ethyl]-4-piperidinyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L13 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:170822 CAPLUS

DOCUMENT NUMBER: 140:417233

TITLE: Synthesis and biological evaluation of 2-(4-fluorophenoxy)-2-phenyl-ethyl piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile
 AUTHOR(S): Dorsey, James M.; Miranda, Maria G.; Cozzi, Nicholas V.; Pinney, Kevin G.

CORPORATE SOURCE: Department of Chemistry and Biochemistry and The Center for Drug Discovery, Baylor University, Waco, TX, 76798-7348, USA

SOURCE: Bioorganic & Medicinal Chemistry (2004), 12(6), 1483-1491

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:417233

AB Three new 2-(4-fluorophenoxy)-2-phenyl-Et piperazines, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-piperazine, and 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(3-trifluoromethylphenyl)-piperazine, modeled after the potent antidepressant fluoxetine and coupled with several functionalized piperazines, have been prepared by chemical synthesis as selective serotonin reuptake inhibitors (SSRIs) with a potentially improved adverse reaction profile. Typical SSRIs, although very effective in the treatment of depression, still face the troublesome side effect of sexual dysfunction. A number of pharmacol. agents-notably, drugs in the piperazine class-have been used to reverse SSRI-induced sexual dysfunction, and evidence for developing an improved SSRI by coupling a fluoxetine congener with the pharmacophore of a reversal agent holds promise. Preliminary data indicates that the hydrochloride (HCl) salts of piperazines exhibit single-site binding at the site of the serotonin reuptake transporter (SERT). However, each of the three compds. are much less potent than typical SSRIs, showing micromolar (μM) affinity for the SERT with IC_{50} values of 1.45 μM , 3.27 μM , and 9.56 μM , resp. Further biol. evaluation of piperazine compds. is needed before definitive conclusions can be made with regard to each compound's potential for use as an SSRI-type candidate which is devoid of sexual side effects. Nevertheless, the initial findings are quite encouraging, thus lending credence to the idea of hybridizing an SSRI congener with that of the pharmacophore of an agent known to reverse or treat SSRI-induced sexual dysfunction.

IT 691872-62-5P 691872-64-7P 691872-66-9P

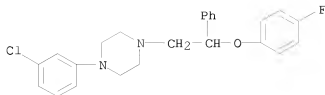
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-62-5 CAPLUS

CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]-, hydrochloride (1:1) (CA INDEX NAME)

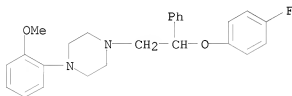
10/513699



● HCl

RN 691872-64-7 CAPLUS

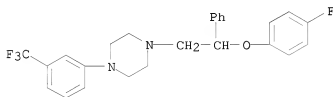
CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 691872-66-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

IT 691872-56-7P 691872-58-9P 691872-60-3P

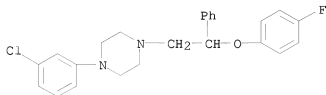
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and structure-activity relationship of 2-(4-fluorophenoxy)-2-Ph-Et piperazines as serotonin-selective reuptake inhibitors with a potentially improved adverse reaction profile)

RN 691872-56-7 CAPLUS

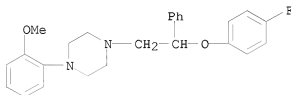
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CN Piperazine, 1-(3-chlorophenyl)-4-[2-(4-fluorophenoxy)-2-phenylethyl]- (CA INDEX NAME)



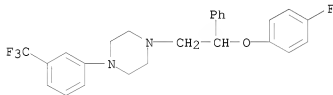
RN 691872-58-9 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-(2-methoxyphenyl)- (CA INDEX NAME)



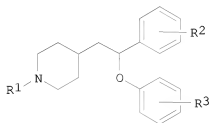
RN 691872-60-3 CAPLUS

CN Piperazine, 1-[2-(4-fluorophenoxy)-2-phenylethyl]-4-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:860624 CAPLUS
 DOCUMENT NUMBER: 140:76994
 TITLE: Syntheses and Binding Studies of New
 [(Aryl)(aryloxy)methyl]piperidine Derivatives and
 Related Compounds as Potential Antidepressant Drugs
 with High Affinity for Serotonin (5-HT) and
 Norepinephrine (NE) Transporters
 AUTHOR(S): Orjales, Aurelio; Mosquera, Ramon; Toledo, Antonio;
 Pumar, M. Carmen; Garcia, Nefitali; Cortizo, Lourdes;
 Labeaga, Luis; Innerarity, Ana
 CORPORATE SOURCE: Research Department, FAES FARMA S. A., Leioa, Vizcaya,
 48940, Spain
 SOURCE: Journal of Medicinal Chemistry (2003), 46(25),
 5512-5532
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:76994
 GI



AB In a wide search program toward new, efficient, and fast-acting antidepressant drugs, series of new compds. having an (aryl)(aryloxy)methyl moiety linked directly or through a methylene chain to different substituted and unsubstituted cycles (isoquinoline, piperazine, piperidine, tetrahydropyran, or cyclopentane) were prepared. These compds. have been evaluated for their affinities for serotonin (5-HT) transporter (SERT) and 5-HT1A and 5-HT2A receptors. Racemic mixts. of 4-[(aryl)(aryloxy)methyl]piperidines I (R1 = H, Me, MeCO; R2 = H, 3-F, 4-F, 4-Cl, 4-Me; R3 = H, 2-CN, 4-O2N, 4-MeO, 2-Ph, etc.) showed much higher affinity values for SERT than fluoxetine and resulted in lack of affinity for 5-HT1A and 5-HT2A receptors. Some of these racemic mixts. were resolved to their enantiomers and tested for binding to norepinephrine (NE) transporter (NET), dopamine (DA) transporter (DAT), and $\alpha 2$ receptor. Several of these enantiomers, (-)-I (R1 = R2 = H; R3 = 2-F), (-)-I (R1 = R2 = H; R3 = 3-F), (-)-I (R1 = H; R2 = 3-F; R3 = 2-F), (+)-I (R1 = H; R2 = R3 = 3-F), displayed a dual binding profile with affinities for SERT and NET with $K_i < 25$ nM and a NET/SERT ratio < 10 . (-)-I (R1 = R2 = H; R3 = 3-F) (coded as F-98214-TA for development studies) showed a dual binding profile with very high affinity values for SERT and NET ($K_i = 1.9$ and 13.5 nM, resp.), and further pharmacol. characterization is in progress for its evaluation as a antidepressant.

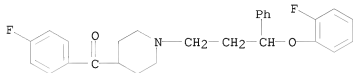
IT 639467-63-3P

10/513699

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of [(aryl)(aryloxy)alkyl]piperidines and analogs as potential antidepressants with high affinity for serotonin and norepinephrine transporters)

RN 639467-63-3 CAPLUS

CN Methanone, [1-[3-(2-fluorophenoxy)-3-phenylpropyl]-4-piperidinyl](4-fluorophenyl)-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2001:636031 CAPLUS

DOCUMENT NUMBER: 135:210828

TITLE: Preparation of novel phenylheteroalkylamines as inhibitors of nitric oxide synthase

INVENTOR(S): Birkinshaw, Tim; Cheshire, David; Mete, Antonio

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.

SOURCE: PCT Int. Appl., 88 pp.

CODEN: PIXXD2

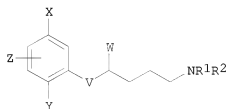
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062713	A1	20010830	WO 2001-SE370	20010220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001034313	A	20010903	AU 2001-34313	20010220
EP 1263714	A1	20021211	EP 2001-906490	20010220
EP 1263714	B1	20040428		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003523992	T	20030812	JP 2001-561723	20010220
AT 265422	T	20040515	AT 2001-906490	20010220
US 20030105161	A1	20030605	US 2002-204815	20020822
US 6743939	B2	20040601		
PRIORITY APPLN. INFO.:			GB 2000-4149	A 20000223
			WO 2001-SE370	W 20010220
OTHER SOURCE(S): MARPAT 135:210828				
GI				



I

AB The title compds. [I; X, Y = alkyl, alkoxy, halo, etc.; Z = H, F; V = O, SOn, NR3; W = alkyl, alkenyl, Ph, etc.; R1, R2 = H, alkyl, cycloalkyl, etc.; NR1R2 = (un)substituted 4-8 membered saturated azacyclic ring optionally

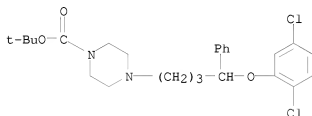
incorporating one further heteroatom selected from O, S or NR8, 5-membered aromatic azacyclic ring optionally incorporating one further N atom; R3 = H, alkyl; R8 = H, alkyl, etc.; n = 0-2] and their pharmaceutically acceptable salts which are inhibitors of nitric oxide synthase and are thereby particularly useful in the treatment or prophylaxis of inflammatory disease and pain, were prepared. E.g., a 4-step synthesis of (1R)-1,oxalate [X = Cl; Y = CN; Z = H; V = O; W = Ph; R1 = H; R2 = Me] was given. The exemplified compds. I (with the exception of one) showed IC50 of < 40 µM against nitric oxide synthase.

IT 357443-66-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel phenylheteroalkylamines as inhibitors of nitric oxide synthase)

RN 357443-66-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[4-(2,5-dichlorophenoxy)-4-phenylbutyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



REFERENCE COUNT:

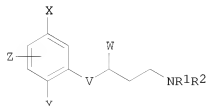
13

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:636023 CAPLUS
 DOCUMENT NUMBER: 135:210827
 TITLE: Preparation of phenylheteroalkylamines as inhibitors
 of nitric oxide synthase
 INVENTOR(S): Cheshire, David; Connolly, Stephen; Cox, David;
 Hamley, Peter; Mete, Antonio; Pimm, Austen
 PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
 SOURCE: PCT Int. Appl., 135 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001062704	A1	20010830	WO 2001-SE373	20010220
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2397234	A1	20010830	CA 2001-2397234	20010220
BR 2001008613	A	20021112	BR 2001-8613	20010220
EP 1263711	A1	20021211	EP 2001-906492	20010220
EP 1263711	B1	20041215		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003523988	T	20030812	JP 2001-561714	20010220
AT 284860	T	20050115	AT 2001-906492	20010220
AU 781141	B2	20050505	AU 2001-34315	20010220
CN 1235870	C	20060111	CN 2001-805489	20010220
NZ 520107	A	20060224	NZ 2001-520107	20010220
NO 2002004014	A	20020925	NO 2002-4014	20020822
MX 2002008203	A	20021129	MX 2002-8203	20020822
US 20030158185	A1	20030821	US 2002-204742	20021018
US 6887871	B2	20050503		
PRIORITY APPLN. INFO.:			GB 2000-4153	A 20000223
			WO 2001-SE373	W 20010220

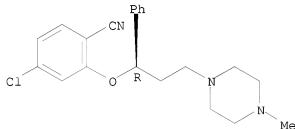
OTHER SOURCE(S): MARPAT 135:210827
 GI



I

- AB The title compds. [I; X, Y = alkyl, alkoxy, halo, etc.; Z = H, F; V = O; W = (un)substituted Ph, 5-6 membered aromatic heterocyclic ring containing 1-3 heteroatoms selected from O, S and N; R1, R2 = H, alkyl, cycloalkyl, etc.; or NR1R2 = (un)substituted 4-8 membered saturated azacyclic ring optionally incorporating one further heteroatom selected from O, S or NR8, 5-membered aromatic azacyclic ring optionally incorporating one further N atom; R8 = H, alkyl, etc.] and their pharmaceutically acceptable salts which are inhibitors of the enzyme nitric oxide synthase and are thereby particularly useful in the treatment or prophylaxis of inflammatory disease, were prepared. Thus, protecting α -(2-aminoethyl)benzenemethanol with di-tert-Bu dicarbonate followed by reacting the resulting carbamate with 4-chloro-2-hydroxybenzonitrile in the presence of triphenylphosphine and di-Et diazodicarboxylate in PhMe/THF, and deprotection of the amine afforded I.HCl [X = Cl; Y = CN, Z = H; V = O; W = Ph; R1, R2 = H]. The exemplified compds. I showed IC50 of < 25 μ M against nitric oxide synthase.
- IT 357401-87-7P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of phenylheteroalkylamines as inhibitors of nitric oxide synthase)
- RN 357401-87-7 CAPLUS
- CN Benzonitrile, 4-chloro-2-[(1R)-3-(4-methyl-1-piperazinyl)-1-phenylpropoxy]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry.

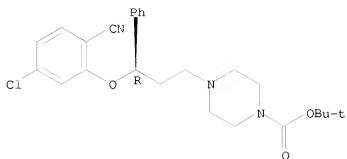


●2 HCl

- IT 357405-84-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of phenylheteroalkylamines as inhibitors of nitric oxide synthase)
- RN 357405-84-6 CAPLUS
- CN 1-Piperazinecarboxylic acid, 4-[(3R)-3-(5-chloro-2-cyanophenoxy)-3-phenylpropyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

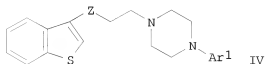
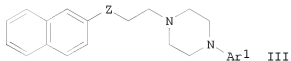
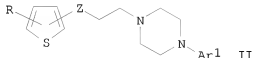
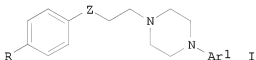
Absolute stereochemistry.

10/513699



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:76 CAPLUS
 DOCUMENT NUMBER: 134:207795
 TITLE: New 1-aryl-3-(4-arylpiperazin-1-yl)propane
 derivatives, with dual action at 5-HT1A serotonin
 receptors and serotonin transporter, as a new class of
 antidepressants
 AUTHOR(S): Martinez-Esparza, Javier; Oficialdegui, Ana-M.;
 Perez-Silanes, Silvia; Heras, Begona; Orus, Lara;
 Palop, Juan-A.; Lasheras, Berta; Roca, Joan; Mourelle,
 Marisa; Bosch, Ana; Del Castillo, Juan-C.; Tordera,
 Rosa; Del Rio, Joaquin; Monge, Antonio
 CORPORATE SOURCE: Departments of Medicinal Chemistry and Pharmacology
 Centro de Investigacion en Farmacobiologia Aplicada
 (CIFA), Universidad de Navarra, Pamplona, 31080, Spain
 SOURCE: Journal of Medicinal Chemistry (2001), 44(3), 418-428
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:207795
 GI



AB In a search toward new and efficient antidepressants,
 1-aryl-3-(4-arylpiperazin-1-yl)propane derivs. I (R = H, Ph, MeO, NO2, Z =
 CO, CHOH, CHOR1, R1 = 4-F3CC6H4, 4-MeOC6H4, 3,4-OCH3OC6H3, Ar1 =

2-MeOC6H4, 4-ClC6H4, 2-pyridyl, etc.), II (R = H, 2,5-Me2, 5-Me, 5-NO2, Z = CO, CNOH, CHOH, CHOR1, R1 = 4-F3CC6H4, 3,4-OCH2OC6H3, 1-ClOH7, position = 2, 3), III and IV (Ar1 = 2-MeOC6H4, 4-ClC6H4, 2-HOC6H4, Z = CO, CHOH) were designed, synthesized, and evaluated for 5-HT reuptake inhibition and 5-HT1A receptor antagonism. This dual pharmacol. profile should lead, in principle, to a rapid and pronounced enhancement in serotonergic neurotransmission and consequently to a more efficacious treatment of depression. The design was based on coupling structural moieties related to inhibition of serotonin reuptake, such as γ -phenoxypropylamines, to arylpiperazines, typical 5-HT1A ligands. In binding studies, several compds. showed affinity at the 5-HT transporter and 5-HT1A receptors. Antidepressant-like activity was initially assayed in the forced swimming test with those compds. with $K_i < 200$ nM in both binding studies. Functional characterization was performed by measuring the intrinsic effect on rectal temperature in mice and also the antagonism to 8-OH-DPAT-induced hypothermia. The most efficacious compds. II (R = H, Z = CHO-1-ClOH7, position = 3, Ar1 = 2-MeOC6H4) (V), II[R = 5-Me, Z = (E)-CNOH, position = 2, Ar1 = 2-MeOC6H4] and IV (Z = CO, CHOH, Ar1 = 2-MeOC6H4) (VI) were further explored for their ability to antagonize 8-OH-DPAT-induced inhibition of forskolin-stimulated cAMP formation in a cell line expressing the 5-HT1A receptor. Furthermore, the antidepressant-like properties of V and VI, which exhibited 5-HT1A receptor antagonistic property in the latter study, were also evaluated in the learned helplessness test in rats. Among these three compds., VI (Z = CHOH) (1-benzo[b]thiophene-3-yl)-3-[4-(2-methoxyphenyl)-1-ypropan-1-ol] showed the higher affinity at both the 5-HT transporter and 5-HT1A receptors ($K_i = 20$ nM in both cases) and was also active in the other pharmacol. tests. Such a pharmacol. profile could lead to a new class of antidepressants with a dual mechanism of action and a faster onset of action.

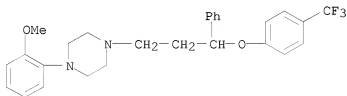
IT 328248-11-9P 328248-15-3P 328248-21-1P
328248-23-3P 328248-24-4P 328248-26-6P
328248-30-2P 328248-33-5P 328248-36-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, 5-HT1A serotonin receptor antagonist and serotonin transporter activity, and structure-activity relationship of aryl(arylpiperazinyl)propanes)

RN 328248-11-9 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

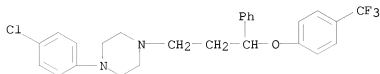


● 2 HCl

10/513699

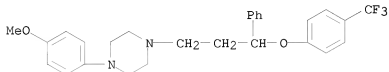
RN 328248-15-3 CAPLUS

CN Piperazine, 1-(4-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



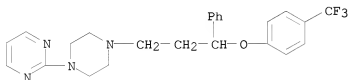
RN 328248-21-1 CAPLUS

CN Piperazine, 1-(4-methoxyphenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



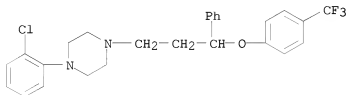
RN 328248-23-3 CAPLUS

CN Pyrimidine, 2-[4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-1-piperazinyl]- (CA INDEX NAME)



RN 328248-24-4 CAPLUS

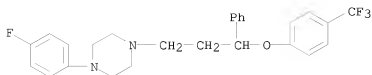
CN Piperazine, 1-(2-chlorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-26-6 CAPLUS

CN Piperazine, 1-(4-fluorophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, hydrochloride (1:2) (CA INDEX NAME)

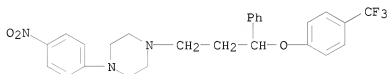
10/513699



● 2 HCl

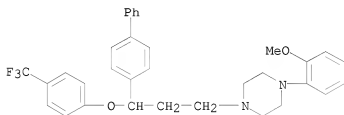
RN 328248-30-2 CAPLUS

CN Piperazine, 1-(4-nitrophenyl)-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)



RN 328248-33-5 CAPLUS

CN Piperazine, 1-[3-[1,1'-biphenyl]-4-yl-3-[4-(trifluoromethyl)phenoxy]propyl]-4-(2-methoxyphenyl)-, hydrochloride (1:2) (CA INDEX NAME)

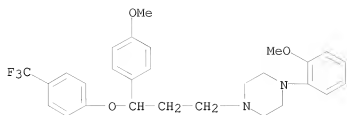


● 2 HCl

RN 328248-36-8 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methoxyphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

10/513699

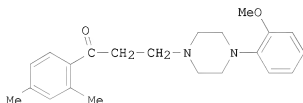


REFERENCE COUNT:

54

THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2000:601312 CAPLUS
 DOCUMENT NUMBER: 133:305272
 TITLE: Design, synthesis and biological evaluation of new 3-[(4-aryl)piperazin-1-yl]-1-arylpropane derivatives as potential antidepressants with a dual mode of action; serotonin reuptake inhibition and 5-HT1A receptor antagonism
 AUTHOR(S): Oficialdegui, A. M.; Martinez, J.; Perez, S.; Heras, B.; Irurzun, M.; Palop, J. A.; Tordera, R.; Lasheras, B.; Del Rio, J.; Monge, A.
 CORPORATE SOURCE: Department of Medicinal Chemistry, Centro de Investigacion en Farmacobiologia Aplicada (CIFA), Universidad de Navarra, Pamplona, 31080, Spain
 SOURCE: Farmaco (2000), 55(5), 345-353
 CODEN: FRMCE8; ISSN: 0014-827X
 PUBLISHER: Elsevier Science S.A.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 133:305272
 GI



I

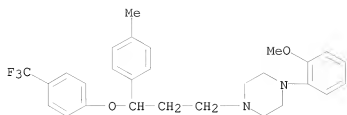
AB It has been suggested that the combination of a selective serotonin reuptake inhibitor (SSRI) and a 5-HT1A receptor antagonist may facilitate the onset of the SSRIs antidepressant action. Accordingly, we describe the synthesis of a series of new 3-[(4-aryl)piperazin-1-yl]-1-arylpropane derivs. with structural modifications performed in Ar1, Ar2 and Z (Z is different functional groups) to obtain the sought dual activity. Comps. were evaluated for in vitro affinity at 5-HT1A receptors and 5-HT transporter. The antidepressant-like activity of derivs. with the higher affinity was assessed initially using the forced swimming test (FST). Compound 1-(2,4-dimethylphenyl)-3-[(2-methoxyphenyl)piperazin-1-yl]-1-propanone (I) showed the best antidepressant-like activity which was further confirmed in the learned helplessness test.

IT 302561-62-2P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (design, synthesis and antidepressant activity of [(aryl)piperazinyl]arylpropane derivs.)

RN 302561-62-2 CAPLUS

CN Piperazine, 1-(2-methoxyphenyl)-4-[3-(4-methylphenyl)-3-[4-(trifluoromethyl)phenoxy]propyl]- (CA INDEX NAME)

10/513699



REFERENCE COUNT:

42

THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1994:655827 CAPLUS

DOCUMENT NUMBER: 121:255827

ORIGINAL REFERENCE NO.: 121:46707a, 46710a

TITLE: Preparation of (hetero)arylpropanolamine derivatives as cerebral calcium overload blockers

INVENTOR(S): Jakobsen, Palle; Kanstrup, Anders; Lundbeck, Jane Marie

PATENT ASSIGNEE(S): Novo Nordisk A/S, Den.

SOURCE: Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 576766	A1	19940105	EP 1992-610053	19920629

R: GB

PRIORITY APPLN. INFO.: EP 1992-610053 19920629

OTHER SOURCE(S): MARPAT 121:255827

AB XR3(RO)CCR4R5CR6R7NR1R2 [X = Ph optionally substituted with one or more cyano, halo, haloalkyl, alkoxy, alkyl, alkanoyl, alkenyl, aryloxy, aralkoxy, amino, alkyl mono or disubstituted amino, alkanoylamino, carbamoyl, alkyl mono- or disubstituted carbamoyl, alkyl substituted with amino, alkyl mono or disubstituted amino, NO₂, morpholino, imidazolyl; R = 3,4-methylenedioxypheyl, aryl or heteroaryl all of which can be optionally substituted with one or more cyano, halogeno, alkyl, alkoxy, alkenyl, trifluoromethyl, alkylene, aryloxy, aralkoxy, alkylthio; R₁, R₂ = alkyl, cycloalkyl, alkenyl, cycloalkylalkyl, all of which can be unsubstituted or substituted with alkyl, alkoxy or cyano; R₁R₂ = 5-, 6- or 7-membered ring containing ≥1 N atom, or which optionally contains 2 N atoms, one or 2 O atom(s) or one or 2 S atom(s) or a combination thereof, which ring is optionally substituted with alkyl, alkoxy, or aryl; and R₃-R₇ = H, alkyl, phenyl; R₄X = carbocyclic ring containing 5 or 6 atoms; or salts thereof with a pharmaceutically acceptable acid; with provisos], were prepared Thus, 1-(4-cyanophenyl)-3-piperidinylpropan-1-ol was condensed with 4-trifluoromethylbenzotrifluoride using KOCMe₃ to give 1-[3-(4-cyanophenyl)-3-(4-trifluoromethylphenoxy)propyl]piperidine, isolated as the oxalate. The latter inhibited stimulated uptake of ⁴⁵Ca by rat P2 synaptosomal preps. with IC₅₀ = 2.2 µg/mL, vs. 26 µg/mL for nifedipine. Generic I formulations are given.

IT 158545-83-6P 158545-84-7P 158545-85-8P

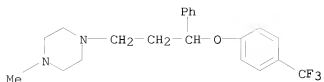
158546-05-5P 158546-06-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as cerebral calcium overload blocker)

RN 158545-83-6 CAPLUS

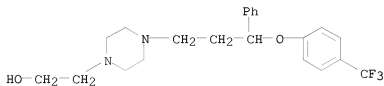
CN Piperazine, 1-methyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-
(CA INDEX NAME)

10/513699



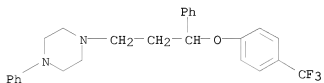
RN 158545-84-7 CAPLUS

CN 1-Piperazineethanol, 4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-
(CA INDEX NAME)



RN 158545-85-8 CAPLUS

CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-
(CA INDEX NAME)



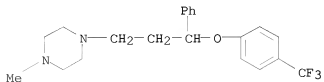
RN 158546-05-5 CAPLUS

CN Piperazine, 1-methyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-,
ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 158545-83-6

CMF C21 H25 F3 N2 O



CM 2

CRN 144-62-7

10/513699

CMF C2 H2 O4



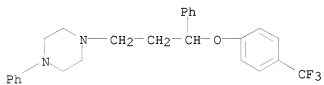
RN 158546-06-6 CAPLUS

CN Piperazine, 1-phenyl-4-[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 158545-85-8

CMF C26 H27 F3 N2 O



CM 2

CRN 144-62-7

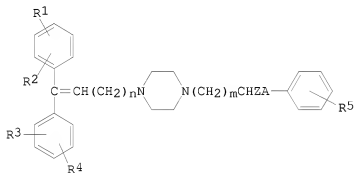
CMF C2 H2 O4



L13 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1989:95279 CAPLUS
 DOCUMENT NUMBER: 110:95279
 ORIGINAL REFERENCE NO.: 110:15755a,15758a
 TITLE: 1-[(1,1-Diphenyl)-1-alkenyl]piperazine derivatives as
 antidepressants and their preparation
 INVENTOR(S): Buzas, Andre; Ollivier, Roland
 PATENT ASSIGNEE(S): Laboratoires Meram, Fr.
 SOURCE: Eur. Pat. Appl., 22 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 288360	A1	19881026	EP 1988-400903	19880414
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
FR 2614021	A1	19881021	FR 1987-5311	19870414
FR 2614021	B1	19910301		
FI 8801633	A	19881015	FI 1988-1633	19880408
NO 8801554	A	19881017	NO 1988-1554	19880411
US 4882331	A	19891121	US 1988-179750	19880411
DK 8802009	A	19881015	DK 1988-2009	19880413
JP 63258862	A	19881026	JP 1988-89163	19880413
CA 1295617	C	19920211	CA 1988-564057	19880413
AU 8814634	A	19881020	AU 1988-14634	19880414
AU 605275	B2	19910110		
ZA 8802633	A	19881228	ZA 1988-2633	19880414
PRIORITY APPLN. INFO.: FR 1987-5311			A	19870414
OTHER SOURCE(S): CASREACT 110:95279; MARPAT 110:95279				

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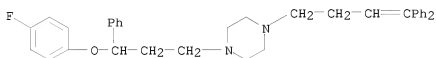
AB The title compds. I [R1-R5 = H, halo, C1-6 alkyl, alkenyl, etc.; n = 1-3; m = 0-3; Z = H, C1-6 alkyl, (substituted) Ph; A = O, CO] and pharmaceutically acceptable salts thereof, useful as antidepressants, were prepared N-Alkylation of 1-(1,1-diphenyl-1-buten-4-yl)piperazine with 2-bromo-1-(4-fluorophenoxy)ethane gave (after treatment with MeSO₃H) gave I. 2MeSO₃H (R1-R4 = H, Z = H, R5 = 4-F, n = 2, m = 1, A = O) (II). II at 18.8 mg/kg i.p. inhibited head twitches induced by 5-hydroxytryptophan in

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mice.
IT 118976-76-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as antidepressant)
RN 118976-76-4 CAPLUS
CN Piperazine, 1-(4,4-diphenyl-3-butenyl)-4-[3-(4-fluorophenoxy)-3-phenylpropyl]-, dimethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 118976-75-3
CMF C35 H37 F N2 O



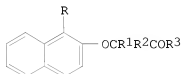
CM 2

CRN 75-75-2
CMF C H4 O3 S



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L13 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:132586 CAPLUS
DOCUMENT NUMBER: 90:132586
ORIGINAL REFERENCE NO.: 90:20867a,20870a
TITLE: Smooth muscle relaxant properties of
2-naphthyl-oxyacetic acid amides
AUTHOR(S): Pestellini, Vittorio; Ghelardoni, Mario; Del Soldato,
Piero; Volterra, Giovanna
CORPORATE SOURCE: Res. Lab., A. Menarini Pharm., Florence, Italy
SOURCE: European Journal of Medicinal Chemistry (1978), 13(5),
486
CODEN: EJMCA5; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

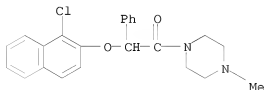


AB Twenty-eight 2-naphthyl-oxyacetamides (I; R = H or Cl; R1 = H or Me; R2 = H, Me, or Ph; R3 = NHR or 4-substituted piperazinyl) were synthesized by reaction of the appropriate amines with the acylchlorides, and were tested for their smooth muscle relaxant properties in vitro and in vivo. Quaternary salts were prepared by treatment of the tertiary bases with MeBr. Structure-biol. activity relations are discussed.

IT 69478-96-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and smooth muscle-relaxant activity of)

RN 69478-96-2 CAPLUS

CN Ethanone, 2-[(1-chloro-2-naphthalenyl)oxy]-1-(4-methyl-1-piperazinyl)-2-phenyl- (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 16:23:34 ON 10 MAR 2009)

L1 FILE 'REGISTRY' ENTERED AT 16:24:30 ON 10 MAR 2009
L2 STRUCTURE UPLOADED

116 S L1 FULL

L3 FILE 'CAPLUS' ENTERED AT 16:25:35 ON 10 MAR 2009
10 S L2 FULL

L4 FILE 'REGISTRY' ENTERED AT 16:27:34 ON 10 MAR 2009
L5 STRUCTURE UPLOADED

6 S L4 FULL

L6 FILE 'CAPLUS' ENTERED AT 16:28:26 ON 10 MAR 2009
6 S L5 FULL

L7 FILE 'REGISTRY' ENTERED AT 16:30:33 ON 10 MAR 2009
L8 STRUCTURE UPLOADED

74 S L7 FULL

L9 FILE 'CAPLUS' ENTERED AT 16:31:15 ON 10 MAR 2009
8 S L8 FULL

L10 FILE 'REGISTRY' ENTERED AT 16:34:04 ON 10 MAR 2009
L11 STRUCTURE UPLOADED

6 S L10 FULL

L12 FILE 'CAPLUS' ENTERED AT 16:35:00 ON 10 MAR 2009
2 S L11 FULL

L13 16 S L12 OR L9 OR L6 OR L3

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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

92.74

843.66

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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STN INTERNATIONAL LOGOFF AT 16:38:02 ON 10 MAR 2009